

ON THE INFLUENCE OF CHEMICAL KINETICS ON THE COMBUSTION OF FUEL DROPLETS

by

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L'INFLUENCE DE LA CINÉTIQUE CHIMIQUE SUR LA COMBUSTION DES GOUTTES

Résumé

L'influence de la cinétique chimique sur la combustion des gouttes est réalisée avec un modèle qui considère symétrie sphérique et les conditions quasi-stationnaires. La cinétique chimique du procès est abordée avec une réaction totale d'ordre n .

Les résultats son exprimés en fonction du produit $p^{n/2} r_g$, p étant la pression, r_g la rayon de la goutte et n l'ordre de la réaction totale. On déduit qu'il existe une valeur minimum de ce produit en dessous duquel une goutte isolée ne peut pas maintenir une flamme.

On a effectué aussi une recherche expérimentale. On a observé la combustion dans l'air à pression variable de gouttes de combustibles suspendues par des fils de quartz très minces. La variation avec le temps du diamètre de la flamme et de la goutte furent obtenus ainsi que les valeurs minimums des diamètre des gouttes pour brûler. On montre que les résultats expérimentaux présentent un accord qualitatif excellent avec ceux de la théorie.

Abstract

The influence of chemical kinetics on the combustion of fuel droplets is studied by means of a theoretical model of the process which considers spherical symmetry and quasi-stationary conditions. Chemical kinetics is approximated by means of an overall reaction rate of n^{th} order.

Results are expressed as a function of the product $p^{n/2} r_g$, where p is the pressure, n the order of the overall reaction and r_g the droplet radius. It is shown that there exists a minimum value of such product under which an individual droplet cannot sustain a flame.

An experimental investigation was also carried out, by burning in air at variable pressure fuel droplets suspended of thin quartz fibres. The laws of variation of both flame and droplet diameter as functions of time were obtained as well as the minimum values of the droplet diameters for combustion as a function of pressure.

It is shown that all experimental results are in excellent qualitative agreement with those predicted by theory.

1. INTRODUCTION

The complex combustion phenomena which take place within the combustion chambers of gas turbines or compression-ignition engines are essentially based on the process of the combustion of a spray of different sized droplets, which are in motion within an oxidizing atmosphere.

Combustion of sprays is studied by means of statistical methods, by applying the laws of the combustion process of individual droplets in a still and oxidizing atmosphere. This process is modified, but not essentially, ^{1,2} by the proximity of other burning droplets (interaction effects) and by the motion of the droplets within the oxidizing atmosphere (forced convection effects).

Combustion of individual droplets has been generally studied by assuming that the chemical reaction rate is infinitely fast. This is the Burke and Schumann hypothesis for studying diffusion flames, which implies that chemical reaction occurs at a zero-thickness layer, where the mass fractions of both fuel and oxidizer become equal to zero. Chemical kinetics is disregarded and results are, then, easily obtained, but it will be shown that this assumption may introduce important errors in the analysis of the process.

On the basis of the aforementioned assumption, it is obtained that the burning rate of the droplets is proportional to the droplet radius and, therefore, that the square of the droplet radius is a linear function of time. It is also obtained that the flame temperature and the flame/droplet radius ratio do not depend on the droplet radius. Another important conclusion is that pressure does not influence the process.

There is available a large experimental evidence on the combustion of droplets. Experimental techniques consisted in observing the combustion of droplets suspended of thin quartz fibres ^{1,2}, or simulating the combustion of liquid droplets by means of porous spheres ^{3,4} to which a controllable fuel flow is supplied. There also exists a few experimental data obtained with ejected and free falling droplets ^{5,6}.

Droplets of practical interest are smaller than 200 μ in diameter, as shown in Fig. 1. It is very difficult to observe the individual combustion of such small droplets. Therefore, the largest part of the available experimental evidence has been obtained with droplets larger than 0.5 mm in diameter. Experimental results obtained with large droplets have been extrapolated for small ones, but it will be shown in this work that such extrapolation is not valid.

The experimental values of the burning rates of large droplets, measured by the slope of curves $r^2 = f(t)$, agreed fairly well with their theoretical values, although Hall and Diederichsen and Bolt ^{5,6} found experimental values for small droplets smaller than those obtained for large droplets.

The theoretical and experimental values of the flame/droplets radius ratio did

**TYPICAL CURVES OF DROPLET
SIZE DISTRIBUTIONS FOR FUEL SPRAYS**

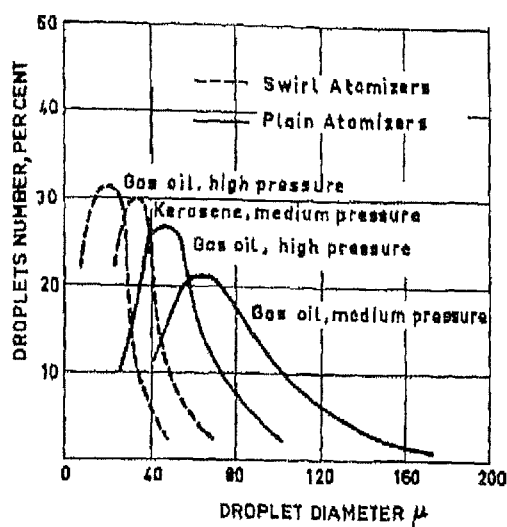


Fig. 1

not coincide, and the experimental values were not constant, but increasing with the droplet radius. Such disagreement was attributed to the influence of free convection, but Kumagai and Isoda found similar laws of variation in a zero-gravity field ^{7,8}. They explained the difference between theoretical and experimental results by means of an approximate theory on transient combustion of droplets. However, transient phenomena alone cannot produce such effects, because Wise, Lorell and Wood ³ found similar laws of variation of the flame/droplet radius ratio for steady-state combustion by using porous spheres of different sizes.

It will be shown that such disagreements between theoretical and experimental results are due to the theoretical model of the process, because the assumption of considering an infinitely fast reaction rate is only strictly applicable when either the droplet radius or the pressure tend towards an infinite value.

There are very few theoretical studies on the combustion of droplets considering finite chemical kinetics. Lorell, Wise and Carr ⁹ studied the problem by taking an overall reaction rate and solving numerically the differential equations of the process. However, they took a constant and rather large value of the droplet radius, they did not consider the influence of pressure and they studied the problem for the case of equal molecular weights of all chemical species. Under such conditions results obtained by assuming an infinite reaction rate are not very different from those derived considering finite chemical kinetics.

At the Instituto Nacional de Técnica Aeronáutica, Madrid, Spain, a research program on combustion has been conducted, part of which comprised the study of the influence of chemical kinetics on the combustion of liquids. In the first place, a general theoretical study was carried out on the combustion of droplets within a reactant atmosphere considering second order chemical kinetics ¹⁰. Afterwards, the

theory was applied to the case of the combustion of bromine droplets in a hydrogen atmosphere ¹¹, considering the actual chemical kinetics of the process.

At the same time an experimental investigation was performed. The investigation consisted in observing the combustion of bromine and nitric acid droplets in hydrogen ¹¹ at variable pressure and in observing the combustion of several types of fuel droplets in air at low pressure.

This investigation was performed in order to verify the theoretical conclusions and in order to obtain some practical data which might be applied to the study of the combustion of fuel sprays.

In the present work a brief résumé of the theoretical study of the combustion of droplets considering finite chemical kinetics will be included, as well as the principal results which have been obtained. Experimental results obtained by burning fuel droplets in air at variable pressure will also be included, as well as a qualitative comparison between theoretical and experimental results.

It will be shown that chemical kinetics influences decisively the process at low pressure or for small droplets and that the assumption of considering an infinitely fast reaction rate is an asymptotic solution of the process, which is the limiting case of the actual solution of the problem when either the pressure or the droplet radius tend towards infinity.

An important conclusion of the theoretical study considering finite chemical kinetics is that there exist minimum values of either the pressure or the droplet radius under which an individual droplet cannot sustain a flame. This interesting conclusion has been experimentally confirmed.

2. FUNDAMENTAL ASSUMPTIONS AND GENERAL EQUATIONS*)

The theoretical treatment of the process is based on the following assumptions:

The droplets are considered to be isolated and at rest, and the process is assumed to have spherical symmetry. Therefore, the influence of natural convection is disregarded. The process is stationary. Under such conditions the study is only strictly applicable to the combustion of constant radius droplets fed with a fuel flow equal to the amount of fuel which is evaporated and burned.

However, it has been shown that for large or medium sized droplets the errors introduced by considering steady-state conditions are not important. This is due to the fact that radial velocity of the droplet surface is small as compared to the diffusion velocities of the species. For this reason, results obtained by using porous spheres of constant diameters are similar to those obtained by burning real liquid droplets.

In order to obtain general conclusions, only reactant species and reaction products will be considered, and the actual chemical kinetics of the process will be approximated by means of an over-all reaction of second order. However, the analytical

*) This résumé of the theoretical treatment of the process has been taken from references 10 and 12.

method used to solve the problem is applicable to more complicated kinetic schemes.

For simplicity, average values will be adopted for the thermal conductivity and for the specific heat of the mixture. The gas pressure will be considered constant throughout the process and the heat transferred to the droplet surface through radiation will be neglected.

Under the aforementioned assumptions the general equations of the process are as follows:

a. Continuity

If w_i is the reaction rate, ε_i the flux fraction of species i , \dot{m} the droplet burning rate and r the radius, we have for each chemical species:

$$\frac{\dot{m}}{4 \pi r^2} \frac{d \varepsilon_i}{dr} = w_i \quad (1)$$

If ν_R and ν_P are the stoichiometric coefficients of the reactants and products of the over-all reaction, and M_R and M_P the molecular masses, we have:

$$\frac{w_R}{\nu_R M_R} = - \frac{w_P}{\nu_P M_P} \quad (2)$$

and through equation (1), it is obtained:

$$\frac{\varepsilon_R - \varepsilon_{Rs}}{\nu_R M_R} = - \frac{\varepsilon_P - \varepsilon_{Ps}}{\nu_P M_P} \quad (3)$$

or else:

$$\frac{\varepsilon_{R\infty} - \varepsilon_{Rs}}{\nu_R M_R} = - \frac{\varepsilon_{P\infty} - \varepsilon_{Ps}}{\nu_P M_P} \quad (4)$$

b. Energy

If h_i is the specific enthalpy of species i , T the temperature and $\bar{\lambda}$ the average value for the mixture of the thermal conductivity, the equation of energy is given by:

$$\dot{m} \sum_i h_i \varepsilon_i - 4 \pi r^2 \bar{\lambda} \frac{dT}{dr} = cte \quad (5)$$

which expresses that the sum of the fluxes of enthalpy and heat is constant. The value of this constant is obtained by expressing that at the droplet surface the heat transmitted is used in vaporizing the liquid fuel, that is:

$$4 \pi r_s^2 \left(\bar{\lambda} \frac{dT}{dr} \right)_s = m q_l \quad (6)$$

where q_l is the latent heat of evaporation of the fuel.

It results:

$$\dot{m} \left(\sum_i h_i \varepsilon_i - \sum_i h_{is} \varepsilon_{is} + q_1 \right) - 4 \pi r^2 \bar{\lambda} \frac{dT}{dr} = 0 \quad (7)$$

Referring the enthalpies h_i to the standard state h_i^0 in the form:

$$h_i = h_i^0 + c_{pi} (T - T_0), \quad (8)$$

taking an average value \bar{c}_p of the specific heats for the mixture and introducing the heat of reaction q_r by means of relations (4), it is obtained:

$$\dot{m} [- (\varepsilon_P - \varepsilon_{Ps}) q_r + \bar{c}_p (T - T_s) + q_1] - 4 \pi r^2 \bar{\lambda} \frac{dT}{dr} = 0 \quad (9)$$

where q_r is given by:

$$q_r = \frac{1}{\nu_P M_P} \left[\sum_R \nu_R M_R h_R^0 - \sum_P \nu_P M_P h_P^0 \right] \quad (10)$$

c. Diffusion

Assuming that only concentration diffusion exists, we have:

$$\sum_j \frac{Y_j}{M_j} \left[\frac{\dot{m} \bar{c}_p}{4 \pi r^2 \bar{\lambda}} \left(\frac{\varepsilon_j}{Y_j} - \frac{\varepsilon_j}{Y_j} \right) \alpha_{ij} - \frac{1}{Y_i} \frac{dY_i}{dr} + \frac{1}{Y_j} \frac{dY_j}{dr} \right] = 0 \quad (11)$$

where α_{ij} is the Lewis-Semenov number, given by:

$$\alpha_{ij} = \frac{\bar{\lambda}}{\varepsilon \bar{c}_p D_{ij}} \quad (12)$$

and Y_i and D_{ij} are, respectively, the mass fractions and diffusion coefficients.

d. Boundary Conditions

It will be assumed that liquid phase reactions do not exist and that there is only one liquid chemical species. It will also be assumed that the chemical reaction goes to completion at infinity and that the temperature and composition of the atmosphere at infinity are known. Thus, we have:

$$\begin{aligned} r = r_s & \begin{cases} T & = & T_s \\ \varepsilon_{is} & = & 1 \\ \varepsilon_{is} & = & 0 \end{cases} \quad (i \neq 1) \\ r = \infty & \begin{cases} T & = & T_\infty \\ Y_{i|\infty} & = & 0 \rightarrow \varepsilon_{i\infty} = 0 \\ Y_i & = & Y_{i\infty} \end{cases} \end{aligned} \quad (13)$$

There exists one boundary condition in excess of the number of differential equations, which gives the burning rate \dot{m} , or "eigenvalue" of the system.

3. SOLUTION OF THE SYSTEM

Solution of the system is simplified by means of the change of variables:

$$\Theta = \frac{\bar{c}_p}{q_r} \left(T - T_s + \frac{q_l}{\bar{c}_p} \right) \quad (14)$$

$$X = \frac{\bar{c}_p}{4 \pi \bar{\lambda}} \frac{\dot{m}}{r} \quad (15)$$

From which:

$$\frac{d s_i}{d X} = - \frac{\bar{c}_p}{\bar{\lambda}} \frac{X_s^2 r_s^2}{X^4} w_i \quad (16)$$

$$\frac{d \Theta}{d X} = - (\Theta - \varepsilon_p) \quad (17)$$

$$\sum_j \left[\frac{Y_j}{M_j} \left(\frac{\varepsilon_j}{Y_j} - \frac{\varepsilon_i}{Y_i} \right) \alpha_{ij} + \frac{1}{Y_i} \frac{d Y_i}{d X} - \frac{1}{Y_j} \frac{d Y_j}{d X} \right] = 0 \quad (18)$$

where X_s , given by:

$$X_s = \frac{\bar{c}_p}{4 \pi \bar{\lambda}} \frac{\dot{m}}{r_s}, \quad (19)$$

is the new eigenvalue of the system. The boundary conditions are now as follows:

$$\begin{aligned} X = X_s & \begin{cases} \Theta & = & \Theta_s \\ \varepsilon_{is} & = & 1 \\ \varepsilon_{js} & = & 0 \end{cases} \quad (i \neq 1) \\ X = 0 & \begin{cases} \Theta & = & \Theta_\infty \\ Y_{i\infty} & = & \varepsilon_{i\infty} = 0 \\ Y_i & = & Y_{i\infty} \end{cases} \end{aligned} \quad (20)$$

The solution of the problem lies on the integration of the non-linear system of differential equations (16), (17) and (18) with boundary conditions (20). In addition, an expression of w_i as a function of the mass fractions and temperatures should be known.

The laws of variation of the functions ε_i and $d \varepsilon_i / d X$ which were found by means of numerical integration of the equations for several typical cases, suggested the adoption of an approximate analytical integration method. This method is based upon considering a reaction zone of finite thickness and on approaching the law of variation of ε_i within such zone by means of two parabolic curves tangent to each other at point $(\varepsilon_{i\infty} + \varepsilon_{is})/2$ and tangent to the lines $\varepsilon_i = \varepsilon_{i\infty}$ and $\varepsilon_i = \varepsilon_{is}$ at the boundaries of the reaction zone.

The reaction zone is determined by the values of its central point X^* and thickness χ . The maximum value of $d\varepsilon_i/dX$, which will be called ε_i^* , should also be fixed. The values of χ , ε_i^* and X^* are obtained from the system of equations:

$$\left(\frac{d\varepsilon_i}{dX} \right)_{X=X^*} = -\frac{\bar{c}_p}{\lambda} - \frac{X_b^2 r_b^2}{X^4} w_i = \varepsilon_i^* \quad (21)$$

$$\chi \varepsilon_i^* = 2 \int_0^{X_b} \frac{d\varepsilon_i}{dX} dX = 2 (\varepsilon_{ib} - \varepsilon_{i\infty}) \quad (22)$$

$$\left(\frac{d^2\varepsilon_i}{dX^2} \right)_{X=X^*} = 0 \rightarrow X^* w_i^* - 4 w_i^* = 0 \quad (23)$$

In this system w_i^* is the value of $w_i(Y_i, \Theta, X)$ for $X = X^*$, in which Y_i and Θ are obtained by integrating differential equations (17) and (18). This integration is performed by introducing into these equations the following expressions for ε_i :

$$\varepsilon_i = \varepsilon_{i\infty} - \frac{2(\varepsilon_{i\infty} - \varepsilon_{ib})}{\chi^2} \left[X - \left(X^* - \frac{\chi}{2} \right) \right]^2 \left(X^* - \frac{\chi}{2} \leq X \leq X^* \right) \quad (24)$$

$$\varepsilon_i = \varepsilon_{ib} + \frac{2(\varepsilon_{i\infty} - \varepsilon_{ib})}{\chi^2} \left[X^* + \frac{\chi}{2} - X \right]^2 \left(X^* \leq X \leq X^* + \frac{\chi}{2} \right) \quad (25)$$

In regions $0 \leq X \leq X^* - \chi/2$ and $X^* + \chi/2 \leq X \leq X_b$, ε_i is taken constant and equal to $\varepsilon_{i\infty}$ and ε_{ib} respectively.

The integration of equation (17) is straightforward. X_b is obtained by integrating this equation between Θ_b and Θ_∞ . The integration of (18) is more involved, because the equation is not linear. However, when the molecular masses of the species as well as the Lewis-Semenov numbers are equal, equation (18) becomes linear and the integration may readily be performed.

An approximate method was developed¹⁰ to integrate Equations (18) for the general case. This method is based on the series expansion of the expressions for Y_i , assuming that χ is small, which is the case that normally occurs in practice.

Several solutions given by the approximate analytical method were compared to those obtained by the numerical integration of the equations. Comparisons were performed for a wide range of variation of the characteristic parameters of the process and for different reaction rates. These comparisons showed that the approximation furnished by the analytical method was excellent in all practical cases.

4. THEORETICAL RESULTS

Chemical kinetics of the combustion of hydrocarbons is not known. Therefore, in

order to perform a qualitative study on the combustion of fuel droplets in air, the combustion process is approximated by means of a second-order over-all reaction:



and chemical kinetics of the process is, then, approximated by taking for the reaction rate an expression of the form:

$$\frac{w_3}{2M_3} = -\frac{w_2}{M_2} = -\frac{w_1}{M_1} = -B \varrho^2 \frac{Y_1 Y_2}{M_1 M_2} \exp\left(-\frac{E}{RT}\right) \quad (27)$$

where B is the frequency constant and E the activation energy of the over-all reaction.

Expression (27) may be written as follows:

$$w_3 = \frac{2 M_3}{M_1 M_2} Q p^2 Y_1 Y_2 (\Theta - \Theta_0)^{-2} \exp\left(-\frac{\Theta_a}{\Theta - \Theta_0}\right) \quad (28)$$

where Θ_a , Θ_0 and Q are constants given by:

$$\Theta_a = \frac{\bar{c}_p E}{R q_r} \quad (29)$$

$$\Theta_0 = \frac{q_l - \bar{c}_p T_s}{q_r} \quad (30)$$

$$Q = \frac{c_p^2 B}{R q_r} \quad (31)$$

All the principal variables of the process: burning rate \dot{m} , temperature Θ^* , flame radius r^* and maximum temperature Θ_{\max} are obtained as a function of the dimensionless product $\sqrt{A} p r_s$, being:

$$A = \frac{Q \bar{c}_p}{M_3 \lambda} \quad (32)$$

Burning rates are generally measured by the slope of the curves of the square of the droplet radius as a function of time. Such curves are usually approximated by means of straight lines, and the slopes are proportional to X_s , because they are given by:

$$k = -\dot{r}_s^2 = \frac{\dot{m}}{2 \pi \varrho_1 r_s} = \frac{2 \bar{\lambda}}{\bar{c}_p \varrho_1} X_s \quad (33)$$

In Figs. 2, 3 and 4 curves of X_s , Θ^* , Θ_{\max} and r^*/r_s are represented as functions of $\sqrt{A} p r_s$ for several values of Θ_∞ . The solutions corresponding to the case of an infinitely fast reaction rate are also included.

All results lie between two limiting cases: when the product $p r_s$ tends towards infinity, the values for X_s , Θ^* , Θ_{\max} and r^*/r_s tend towards those obtained by assuming an infinite reaction rate.

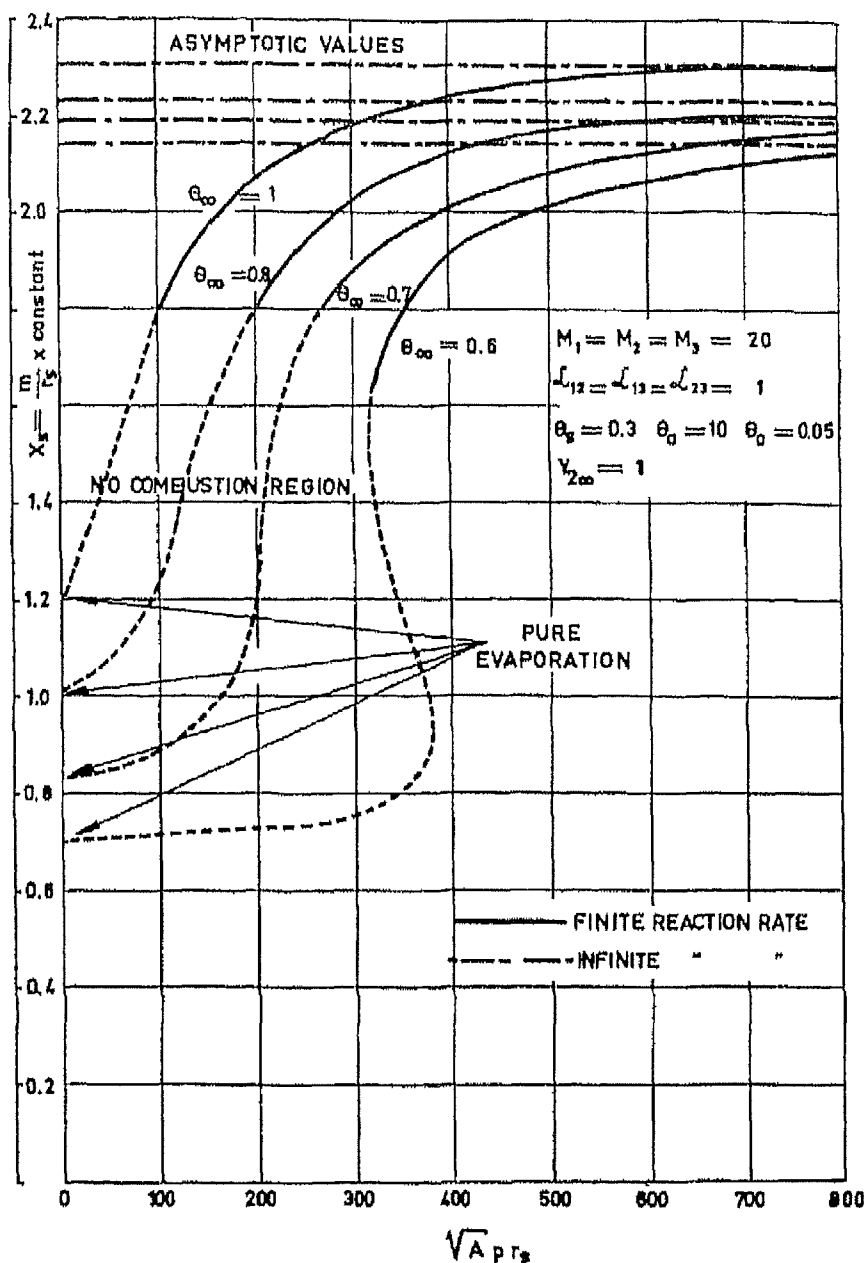


Fig. 2

On the other hand, when $p r_B$ tends towards zero, the value of X_B is given by:

$$X_B = \log \frac{\theta_{\infty}}{\theta_0} \quad (34)$$

θ^* and θ_{\max} tend towards θ_{∞} and r^*/r_B tends towards infinity, all values corresponding to the case of pure evaporation of droplets in absence of combustion.

Parameter θ_0 influences decisively the process. When θ_0 is small, X_B , θ^* , θ_{\max} and r^*/r_B are close to their asymptotic values, even for very small values of $\sqrt{A} p r_B$.

On the contrary, for large values of Θ_a such variables separate from their asymptotic values at large values of $\sqrt{A} p r_s$, and they reach rapidly values very close to those corresponding to $\sqrt{A} p r_s = 0$. (Ref. 10).

An interesting conclusion is that solutions close to the case of pure evaporation do not represent actual combustion processes, since temperature profiles are very flat 10, with maximum temperatures close to Θ_∞ , and reaction zones are very wide. Therefore, theoretical results show that minimum values of either the pressure or the droplet radius exist under which combustion is not possible.

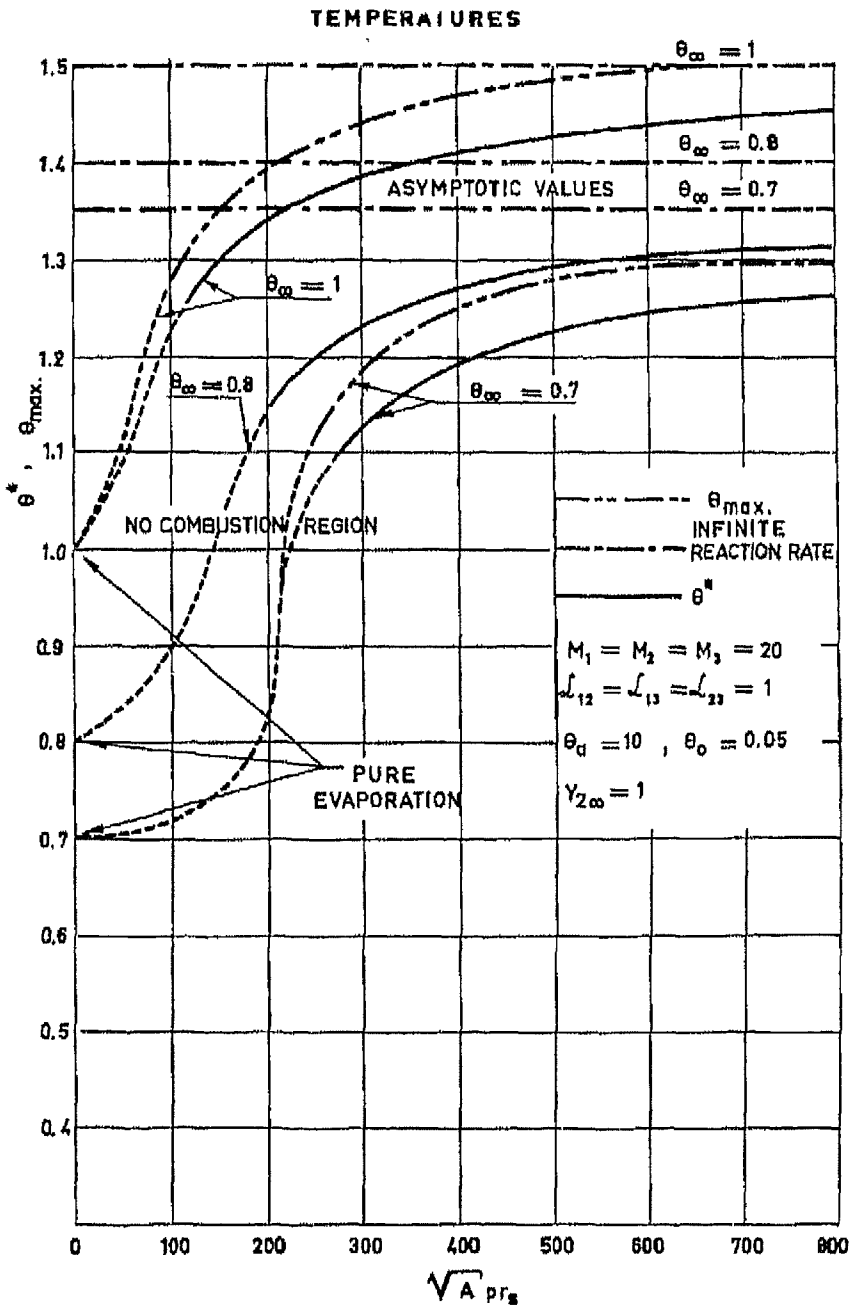
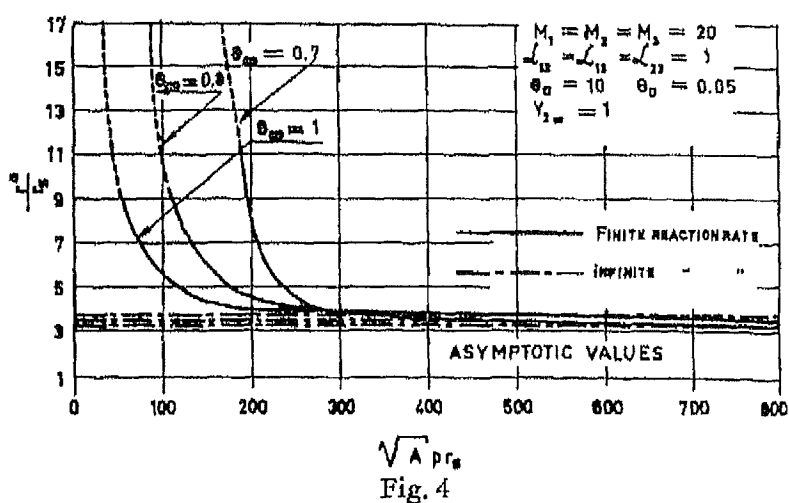
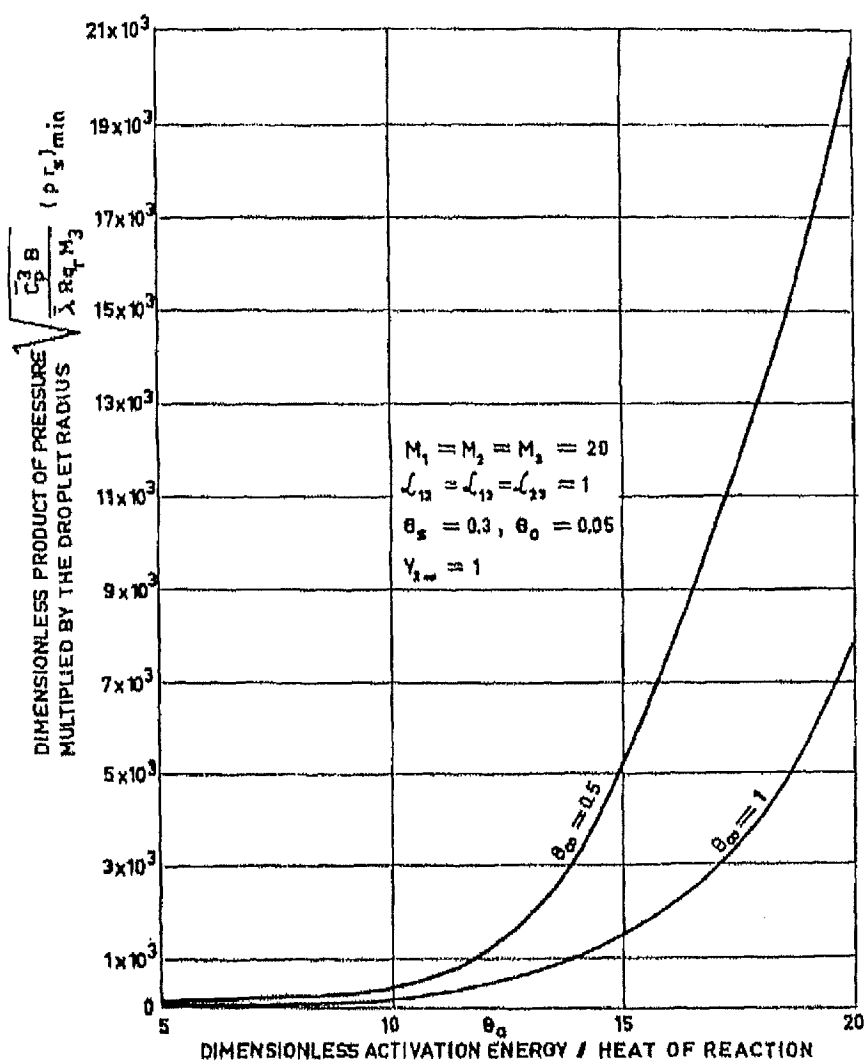


Fig. 3

POSITION OF THE FLAME



MINIMUM DROPLET RADIUS AND PRESSURE FOR COMBUSTION



Variables X_s , Θ^* and r^*/r_s change rapidly from values close to the origin ($\sqrt{A} p r_s = 0$) up to values close to those corresponding to $\sqrt{A} p r_s = \infty$. Therefore, the minimum value of $\sqrt{A} p r_s$ required for combustion may be approximately calculated by taking, for example, the value of $\sqrt{A} p r_s$ corresponding to the average value of X_s between $(X_s)_{\sqrt{A} p r_s = 0}$ and $(X_s)_{\sqrt{A} p r_s = \infty}$. Such minimum values depend strongly on Θ_a , and they are represented in Fig. 5.

In order to verify the aforementioned theoretical conclusions an experimental research program was carried out. The investigation was conducted in two directions: in the first place, combustion of bromine and nitric acid droplets in gaseous hydrogen was observed. Hydrogen was selected, among other reasons, because the influence of chemical kinetics on the combustion process is more important when the molecular mass of the gaseous species surrounding the droplet is smaller than the molecular mass of the liquid species forming the droplet. Results of this research program as well as their comparison with theoretical results have already been published 11, 12.

Another part of the research program was the investigation of the influence of pressure and droplet size on the combustion in air of fuel droplets.

A quantitative agreement between experimental and theoretical results could not be expected, due to the lack of data on chemical kinetics of the combustion of fuels. However, it was expected that at low values of the product $p r_s$ the influence of chemical kinetics should decrease the slope of curves $r_s^2 = f(t)$ and it should also increase the values of the ratio of the flame radius to the droplet radius. Another important objective of the investigation was to obtain the minimum values for combustion of the product $p r_s$.

The experimental technique consisted in observing the combustion of fuel droplets suspended of thin quartz fibres. The droplet size could only be modified within a narrow range (0.2—1 mm in radius). Therefore, the influence of air pressure was the main objective of the investigation.*)

In Fig. 6 the research facility is shown. A steel combustion chamber was used in which air pressures from very small values up to several atmospheres could be established. The chamber has an orifice at its top, which is closed by means of a glass tube which moves up and down driven by an electromagnetic actuator. When the desired pressure is set within the chamber, a droplet suspended from a quartz fibre is introduced into the tube, closing simultaneously the orifice. The tube is then moved downwards and the droplet is ignited by electrodes which are placed in position by the motion of the tube.

Motion pictures of the burning droplets were taken by means of an Akeley

*) Hall and Diederichsen⁵ investigated the influence of pressure on the combustion of fuel droplets. However, in the range of pressures which they considered (from one up to 20 atmospheres) it has almost no influence on the results, because for such conditions results are very close to their asymptotic values. Therefore, they concluded that pressure did not influence appreciably combustion of droplets.

SCHEMATIC DIAGRAM OF APPARATUS

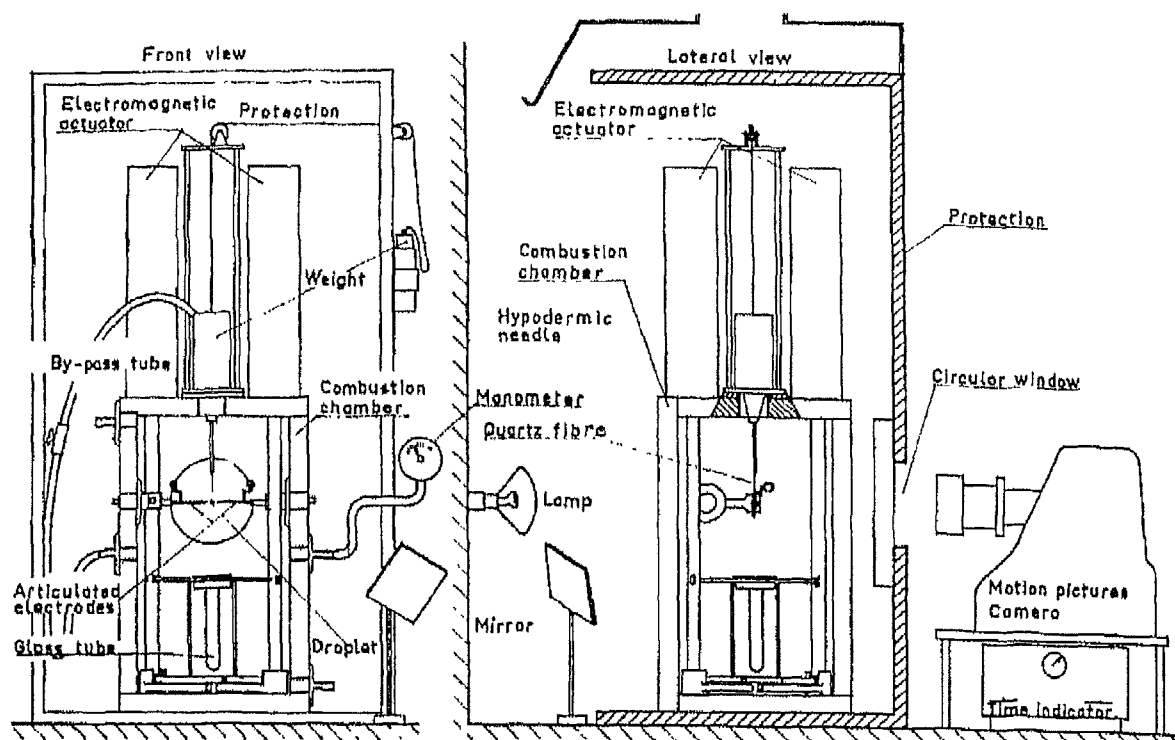


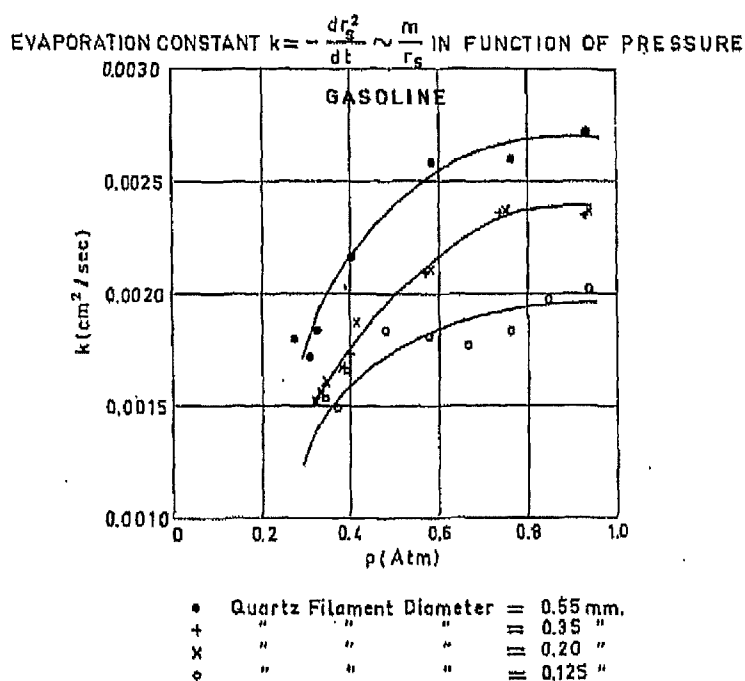
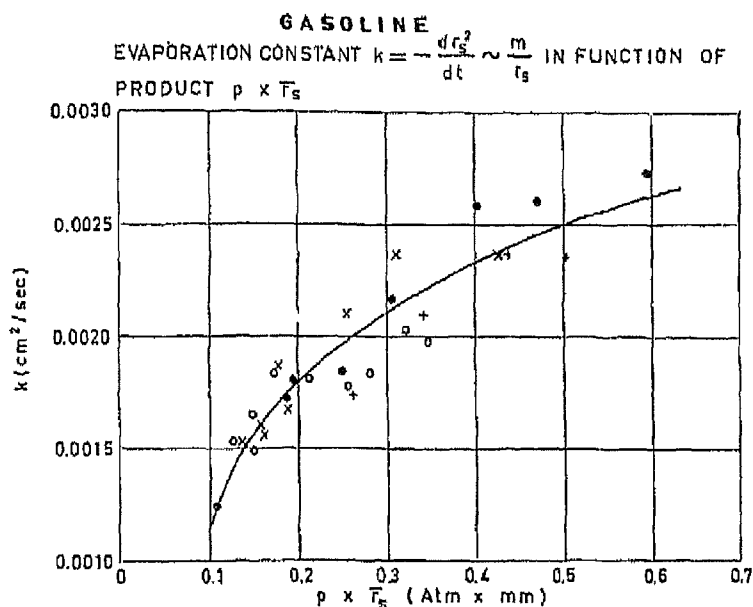
Fig. 6

camera, and the values of both droplet and flame diameters were measured as functions of time. Droplet diameter was taken as the mean value of two perpendicular diameters measured at 45° from the fibre axis. Flame diameter was taken as the value of the maximum horizontal diameter of the flame.

Normal heptane, 100 octane gasoline, RD 2498 kerosene and ethyl alcohol were tested. Pressure was varied for each fuel from the minimum value required to obtain ignition up to a value at which results were sensibly constant (independent of pressure).

Results for gasoline and kerosene are shown in Fig. 7 through 14. It may be observed that the experimental laws of variation of the evaporation constants (proportional to X_g) and of the flame/droplet radius ratio r^*/r_g as functions of the pressure and as functions of the droplet radius agree perfectly well, from a qualitative point of view, with those obtained theoretically. It may be pointed out the excellent correlation of results which is obtained when they are plotted as a function of the product $p r_g$ for gasoline and as a function of $p^{0.55} r_g$ for kerosene.

For large values of either the pressure or the droplet radius, the values of k and r^*/r_g tend towards asymptotic or constant values, and when the pressure or the droplet radius are reduced, k and r^*/r_g decrease up to minimum values of p or r_g under which combustion was not possible. The results confirm the strong influence of chemical kinetics on the process at low pressure or for small droplets and they imply that the assumption of considering an infinitely fast reaction rate is not valid for such conditions.



In Figs. 15 and 16 photographs taken from motion pictures of burning droplets of gasoline are shown. Fig. 15 shows a droplet burning at ambient pressure and Fig. 16 a droplet burning at 1/3 of atmosphere. In this case the flame is darker and its shape is almost spherical; which means that free convection is less important. This, in turn, implies that combustion temperature is lower according to the results theoretically predicted.

In Fig. 17 and 18 minimum values of the droplet radius for combustion r_{80} are shown as a function of the pressure for the four fuels investigated. Such radius r_{80} represents the minimum value for which ignition could not be achieved by means of electric sparks, and sometimes the extinction value of the radius after combustion, of the type shown in Fig. 19.

It may be expected that the ignition mechanism should influence the process and there also is a possible influence of the flame stability on the extinction values of

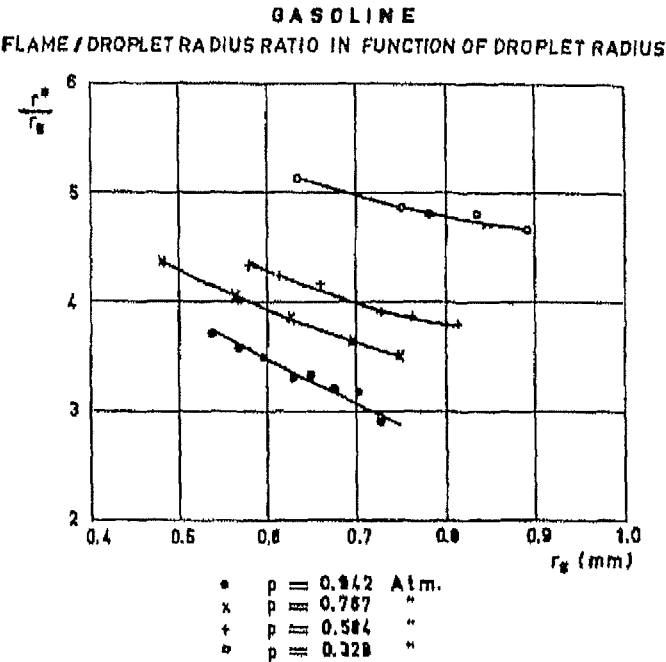


Fig. 9

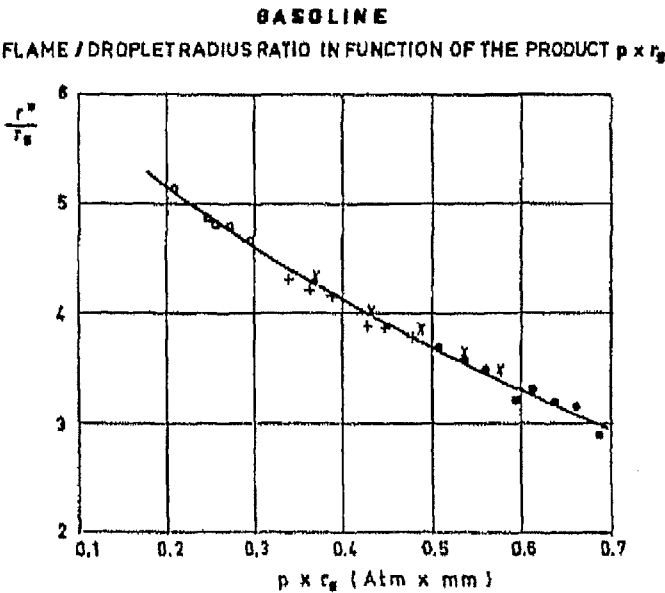


Fig. 10

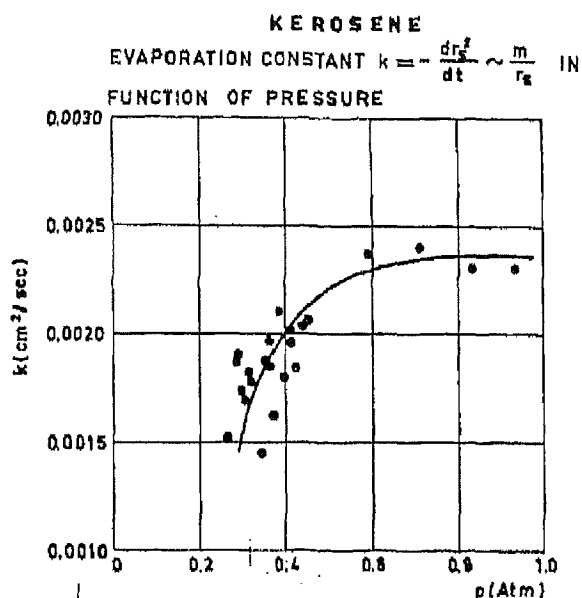


Fig. 11

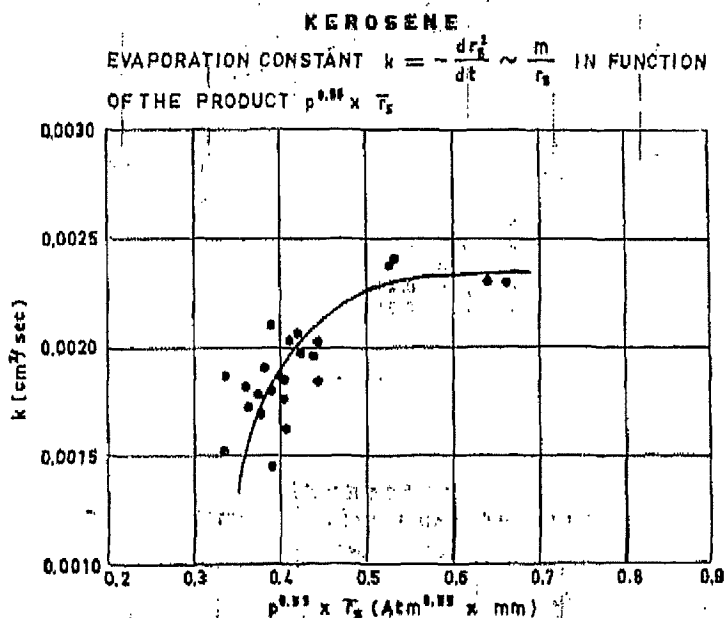


Fig. 12

either the pressure or the droplet radius. These phenomena explain the dispersion of results and they prevented the formulation of any precise law of variation of the extinction radius as a function of pressure. However, approximated results may be obtained from Figs. 18 and 19.

From the results of the investigation it may be concluded that at the working conditions which exist within the combustion chambers of gas turbines or compression-ignition engines, the droplets of their sprays will be under conditions at which chemical kinetics will influence strongly the combustion process. Gas pressure is high, but the droplets are small, to such extent that the product pr_s will probably

have values smaller than those required for disregarding chemical kinetics. It is also possible that for certain conditions the droplets cannot sustain individual flames, and then, the combustion process would consist in the vaporization of the droplets within a common flame.

Therefore, spray combustion cannot be studied by applying the burning laws of individual droplets obtained by assuming an infinitely fast reaction rate, as it has

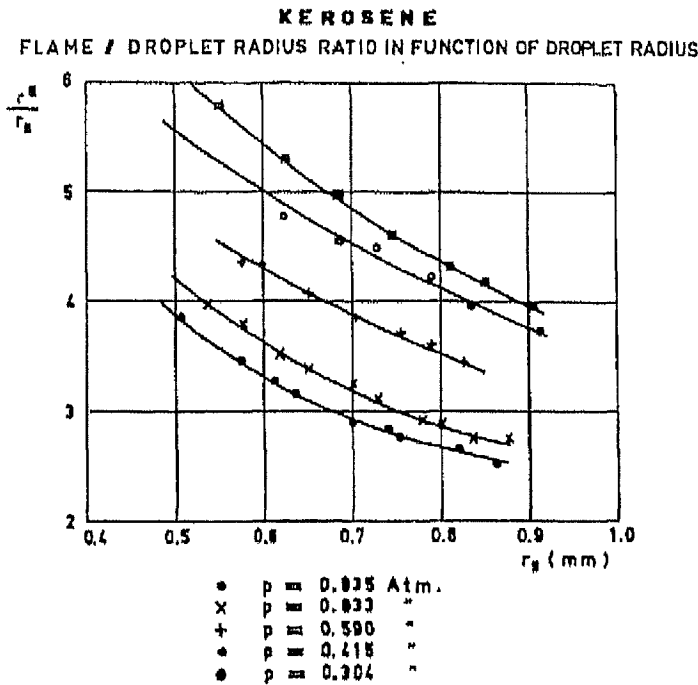


Fig. 13

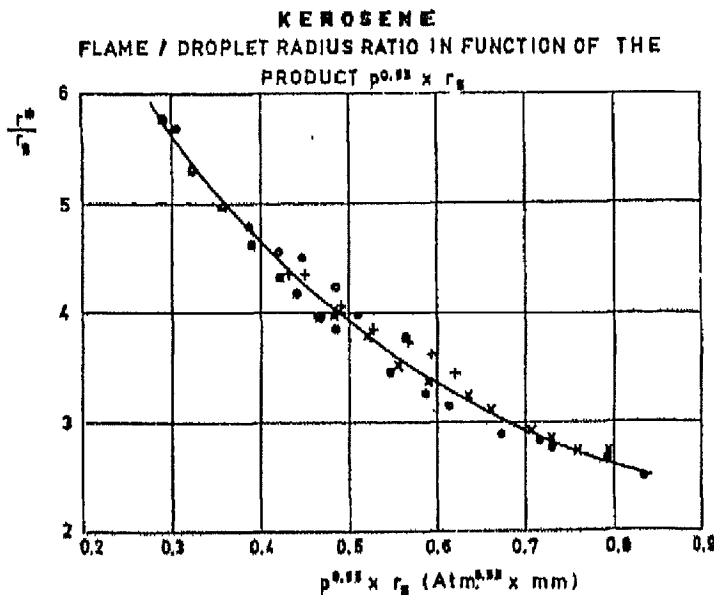


Fig. 14

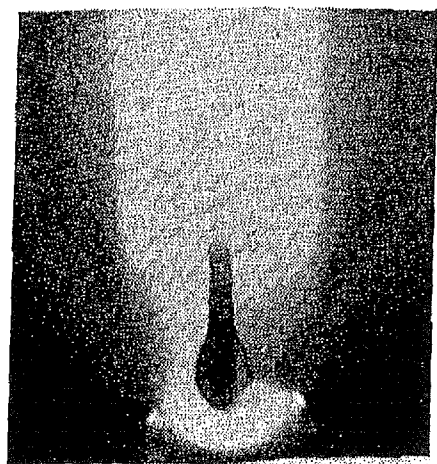


Fig. 15 A
 $t = 0$

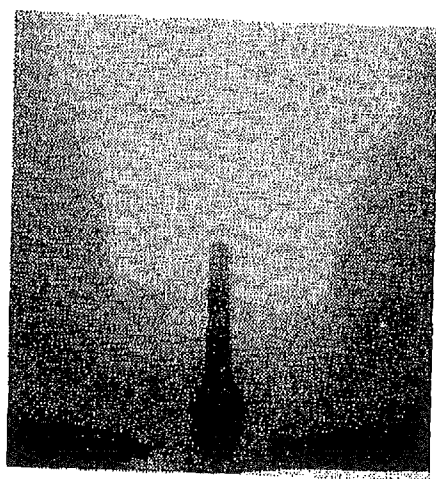


Fig. 15 B
 $t = \frac{1}{8}$ sec.

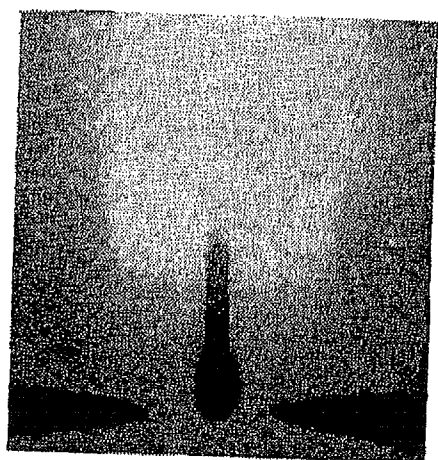


Fig. 15 C
 $t = \frac{2}{8}$ sec.

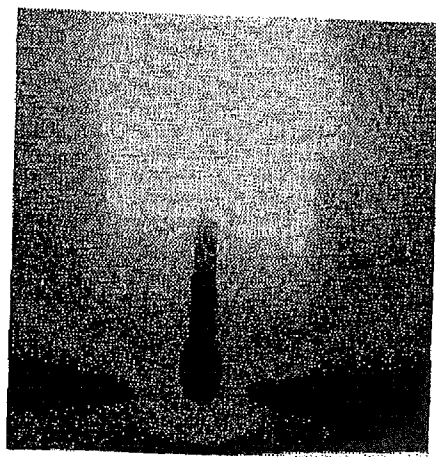


Fig. 15 D
 $t = \frac{3}{8}$ sec.

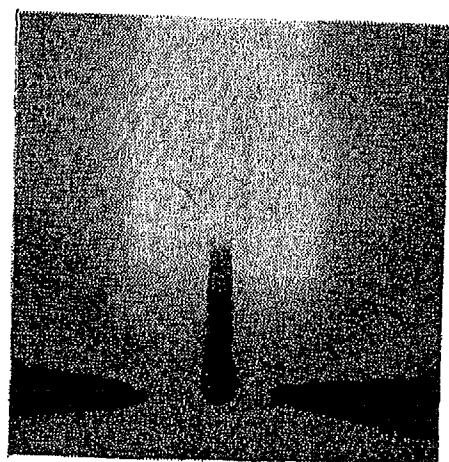


Fig. 15 E
 $t = \frac{4}{8}$ sec.

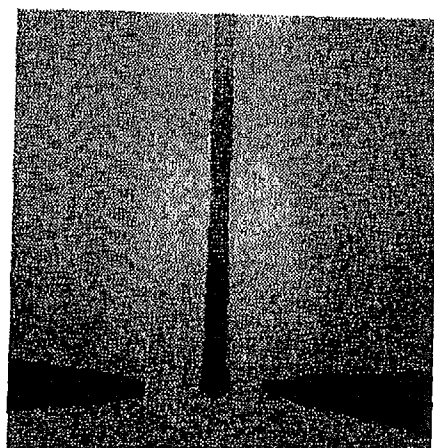


Fig. 15 F
 $t = \frac{5}{8}$ sec.

Fig. 15. A gasoline droplet burning at one atmos.

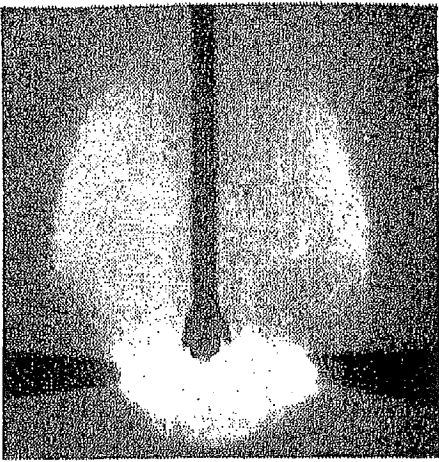


Fig. 16 A
 $t = 0$

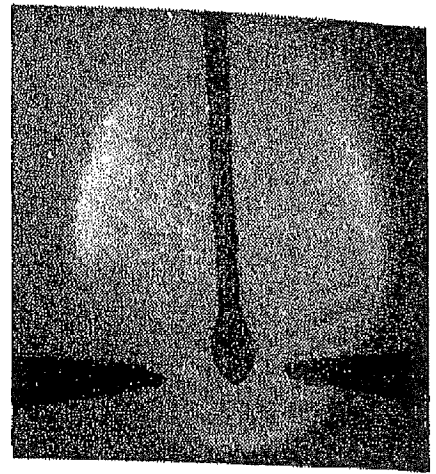


Fig. 16 B
 $t = \frac{1}{4}$ sec.

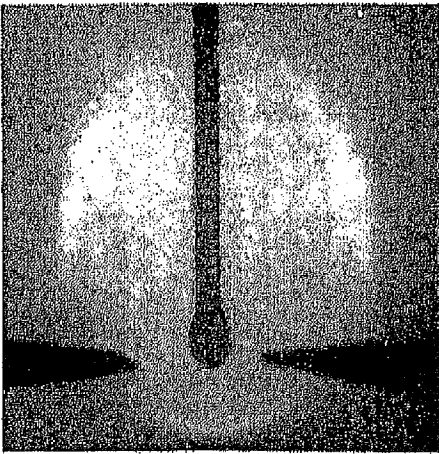


Fig. 16 C
 $t = \frac{2}{4}$ sec.

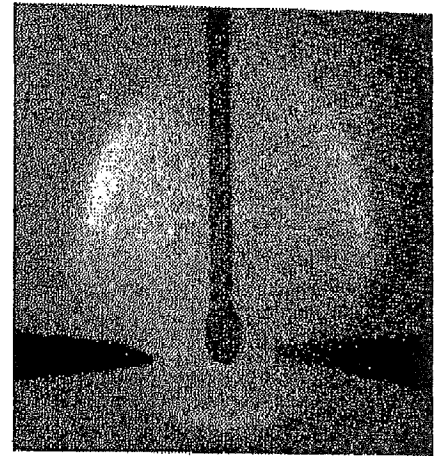


Fig. 16 D
 $t = \frac{3}{4}$ sec.

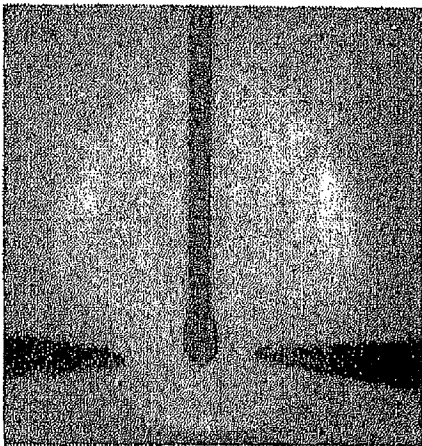


Fig. 16 E
 $t = \frac{4}{4}$ sec.

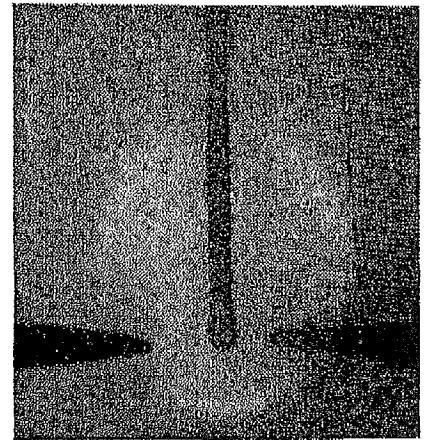


Fig. 16 F
 $t = \frac{5}{4}$ sec.

Fig. 16. A gasoline droplet burning at $\frac{1}{3}$ of atmos.

been customarily done. This might explain some of the discrepancies between theoretical and experimental results which usually are found when studying spray combustion and it also gives an explanation of some results obtained by Graves and

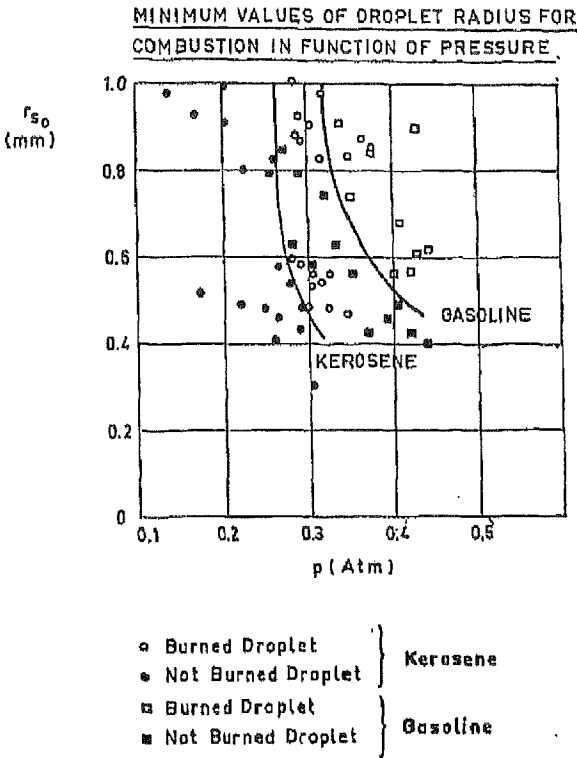


Fig. 17

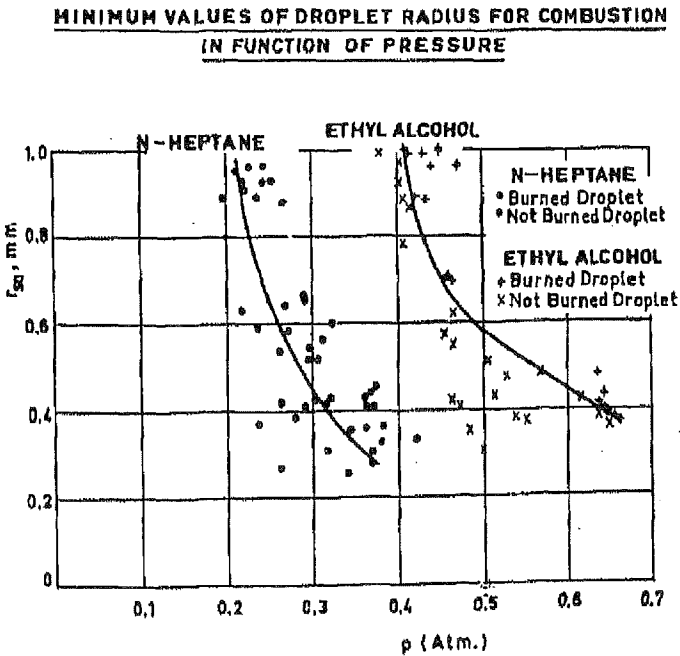


Fig. 18

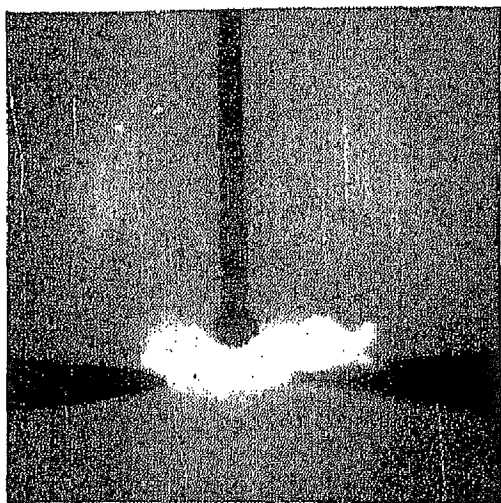


Fig. 19 A
Ignition

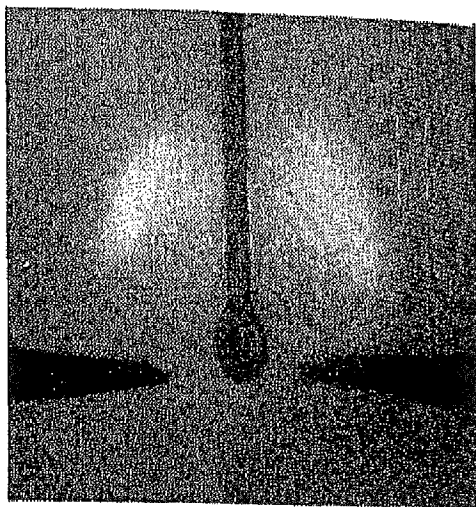


Fig. 19 B
Flame

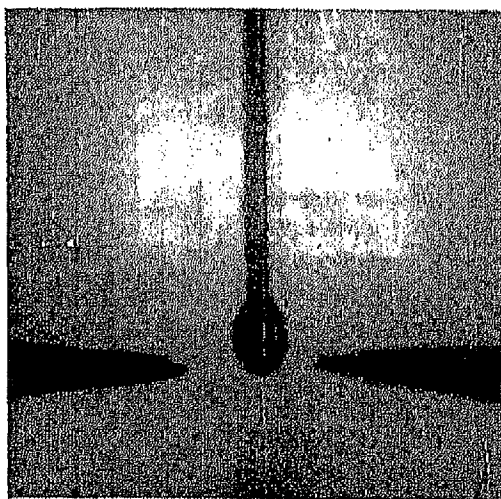


Fig. 19 C
Extinction

Fig. 19. Combustion of a n-heptane droplet near extinction conditions ($p = 1/4$ atmos.)

Gerstein ¹³, who deduced from their experiments that chemical kinetics should influence strongly combustion of sprays.

ACKNOWLEDGMENT*

The author is indebted to Dr. Garcia Moreno for his excellent contribution to the experimental work described in this paper.

Madrid, December, 1961.

* The research reported in this paper has been sponsored in part by the Office of Scientific Research OAR, United States Air Force.

NOTATION

A, Q	Constants of the reaction rate equation.
B	Frequency factor.
c_p	Specific heat at constant pressure.
\bar{c}_p	Average value of c_p for the mixture.
D_{ij}	Diffusion coefficient.
E	Activation energy.
h_i	Specific enthalpy.
k	Evaporation constant.
\dot{m}	Burning rate (mass of fuel burned per unit time).
M_i	Molecular mass.
p	Pressure.
q_l	Latent heat of evaporation.
q_r	Heat of reaction.
r	Radius.
r_s	Droplet radius.
R	Gas constant.
t	Time.
T	Absolute temperature.
w_i	Reaction rate.
X	$= c_p m / 4\pi \bar{\lambda} r$, dimensionless coordinate.
X_s	$= c_p / 4\pi \bar{\lambda} r_s$, eigenvalue of the system, proportional to the evaporation constant
Y_i	Mass fraction.
ε_i	Ratio of flux of mass of species i to total mass flow.
λ	Thermal conductivity.
$\bar{\lambda}$	Average value of λ for the mixture.
$\alpha_{ij} = \bar{\lambda} / \rho D_{ij} c_p$	Lewis-Semenov number.
ν_i	Stoichiometric coefficients of chemical reaction.
ρ	Gas density.
ρ_l	Density of the liquid of the droplet.
Θ	Dimensionless temperature.
Θ_0	Constant.
χ	Reaction zone thickness at the X coordinate system.

SUBSCRIPTS

i, j	Chemical species in general.
R, P	Reactant and products, respectively.
1	Gaseous reactant from the droplet.
2	Oxidizer.
3	Reaction products.
s	On the droplet surface.

SUPERSSCRIPTS

*	Center of the reaction zone. (Point at which $d \varepsilon_i / dX$ is a maximum).
.	Time derivative.
,	Derivative in respect of X .
o	Standard state.

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PRESENTATION BY THE AUTHOR

The influence of chemical kinetics on the combustion of fuel droplets is studied by means of a theoretical model of the process which considers spherical symmetry and quasi-stationary conditions. Chemical kinetics is approximated by means of an overall reaction rate of n^{th} order.

Results are expressed as a function of the product $p^{n/2} r_0$, where p is the pressure, n the order of the overall reaction and r_0 the droplet radius. It is shown that there exists a minimum value of such product under which an individual droplet cannot sustain a flame.

An experimental investigation was also carried out, by burning in air at variable

pressure fuel droplets suspended of thin quartz fibres. The laws of variation of both flame and droplet diameter as functions of time were obtained as well as the minimum values of the droplet diameters for combustion as a function of pressure.

It is shown that all experimental results are in excellent qualitative agreement with those predicted by theory.

DISCUSSION

Dr. *A. E. W. Austen*

May I say first of all that I have the greatest admiration for this work by the author on single droplet combustion. However, I wish to question its significance so far as combustion in diesel engines is concerned, and in particular I want to disagree with the author's conclusion that in diesel engines, at any rate, one cannot neglect reaction kinetics. This is of consequence to us because we habitually do neglect reaction kinetics.

Now, the grounds for disagreement are these: the reaction rates which are arrived at in the paper appear to me to be several orders of magnitude slower than those which apply in diesel engines. Secondly, the one quantity above all others which we found to control reaction rates in diesel engines is gas velocity. Now this, of course, has no opportunity to have any effect in the experiments described by the author. I interpret this as meaning that, in diesel engines, combustion does not occur as single droplets. Our hypothesis is that combustion occurs either by evaporation and mixing prior to ignition, in which case combustion takes place as a pre-mixed flame or, later on in the cycle, by evaporation and then burning at the boundary of a region of fuel vapour or a region rich in fuel vapour, as a diffusion flame. In these circumstances we believe that the major rate-determining process is mixing which, in turn, is controlled by the general level and extent of the turbulence in the gas velocity.

I should like to put the question to the author – does he believe there is anything in his work which conflicts with the hypothesis I have just outlined?

THE AUTHOR'S REPLY

Mr. *Carlos Sanchez Tarifa*

In the first place I want to thank Dr. *Austen* for his comment.

I think I have not mentioned chemical kinetics in connection with Diesel combustion, among other reasons because I am not familiar enough with combustion processes in compression-ignition engines, but I do know that chemical kinetics plays an important role in spray combustion in both gas turbines and liquid propellant rocket engines. However, I may suggest an explanation which answers

the question Dr. *Austen* put to me. In Diesel engines pressure is much higher than in gas turbines. Droplets burning rates increase as $p^{n/2}$, where p is pressure and n is the order of the overall reaction rate. Therefore, at high pressure burning rates have large values and they are close to their asymptotic values obtained by taking an infinitely fast reaction rate. This assumption of taking an infinitely fast reaction rate disregards chemical kinetics, and therefore, this might explain why chemical kinetics could be of secondary importance in the combustion processes of Diesel engines.

I want also to point out one of the main conclusions of the paper in connection with the influence of chemical kinetics. When the droplets are small, or at low pressure, they do not sustain individual flames but they evaporate together within a common flame. This is due to the influence of chemical kinetics and such influence has been theoretically obtained and it has also been experimentally verified by observing spray combustion.